

Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

## Strain-induced phase transformation under compression and compression and torsion in a diamond anvil cell: simulations of a sample and gasket

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### ABSTRACT

Combined high pressure phase transformations (PTs) and plastic flow in a sample within a gasket compressed in diamond anvil cell (DAC) or compressed and twisted in rotational DAC are studied using finite element method (FEM). The key point is that PTs are modeled as strain-induced, which involves a completely different kinetic description than for traditional pressure-induced PTs. Corresponding microscale constitutive model is presented. Contact sliding with Coulomb and plastic friction at the boundaries between the sample, gasket, and anvil is taken into account. A comprehensive computational study of the effects of the kinetic parameter, ratio of the yield strengths of high and low-pressure phases and the gasket, sample radius and initial thickness on the PTs and plastic flow is performed. A new sliding mechanism at the contact line between the sample, gasket, and anvil called extrusion-based pseudoslip is revealed, which plays an important part in producing high pressure. Strain-controlled kinetics explains why experimentally determined PT pressure and kinetics (concentration of high pressure phase versus pressure) differ for different geometries and properties of the gasket and the sample: they provide different plastic strain, which was not measured. Utilization of the gasket changes radial plastic flow toward the center of a sample, which leads to high quasi-homogeneous pressure for some geometry. For transformation to a stronger high pressure phase, plastic strain and concentration of a high-pressure phase are also quasi-homogeneous. This allowed us to suggest a method of determining strain-controlled kinetics from experimentation, which is not possible for weaker and equal-strength high-pressure phases and cases without a gasket. Effect of torsion is studied in detail. Some experimental phenomena are reproduced and interpreted. Developed methods and obtained results represent essential progress toward the understanding of PTs under compression and compression and torsion in the DAC. This will allow one optimal design of experiments and conditions for synthesis of new high pressure phases.